

Development of the NAPAP (National Acid
Precipitation Assessment Program) Emissions
Inventory to Support Applications of the
Eulerian Regional Acid Deposition Model

GCA Corp., Bedford, MA

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Apr 86



U.S. Department of Commerce
National Technical Information Service

NTIS.

DEVELOPMENT OF THE NAPAP EMISSIONS INVENTORY TO SUPPORT
APPLICATIONS OF THE EULERIAN REGIONAL ACID DEPOSITION MODEL

By:

Frederick M. Sellars
GCA Technology Division, Inc.
Bedford, Massachusetts 01730

and

J. David Mobley
Air and Energy Engineering Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

EPA Contract 68-02-3997

AIR AND ENERGY ENGINEERING RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)			
1. REPORT NO. EPA/600/D-86/092		3. RECIPIENT'S ACCESSION NO.	
4. TITLE AND SUBTITLE Development of the NAPAP Emissions Inventory to Support Applications of the Eulerian Regional Acid Deposition Model		5. REPORT DATE April 1986	
7. AUTHOR(S) F. M. Sellars and J. D. Mobley		6. PERFORMING ORGANIZATION CODE	
9. PERFORMING ORGANIZATION NAME AND ADDRESS GCA Technology Division Bedford, Massachusetts 01730		8. PERFORMING ORGANIZATION REPORT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS EPA, Office of Research and Development Air and Energy Engineering Research Laboratory Research Triangle Park, NC 27711		10. PROGRAM ELEMENT NO.	
		11. CONTRACT/GRANT NO. 68-02-3997, Task 13	
		13. TYPE OF REPORT AND PERIOD COVERED Published Paper; 3/86	
		14. SPONSORING AGENCY CODE EPA/600/13	
15. SUPPLEMENTARY NOTES AEERL project officer is J. David Mobley, Mail Drop 61, 919/541-2612. Presented at APCA annual meeting, June 1986, Minneapolis, MN.			
16. ABSTRACT The paper describes the processes and data sources used to develop temporal, spatial, and species allocation factors for the National Acid Precipitation Assessment Program (NAPAP). NAPAP has charged its task group on Emissions and Controls with the development of inventories of acid rain precursor emissions from anthropogenic sources. To support applications of the Eulerian Regional Acid Deposition Model (RADM), the 1980 NAPAP Annual Emissions Inventory was further resolved. Temporal allocation of annual emissions to hourly emissions estimates for a typical weekday, Saturday, and Sunday in each season; spatial allocation of county-level area source and minor point source emissions to 63,000 20 x 20 km grid cells; and species allocation of NOx to NO and NO2, TSP to alkalinity classes, and VOC to 29 photochemical reactivity classes were performed.			
17. KEY WORDS AND DOCUMENT ANALYSIS			
a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Pollution Precipitation (Meteorology) Acidification Assessments Emission	Inventories Euler Equations of Motion Mathematical Models	Pollution Control Stationary Sources NAPAP Acid Rain	13B 15E 04B 12A 07B, 07C 14B 14G
18. DISTRIBUTION STATEMENT Release to Public		19. SECURITY CLASS (This Report) Unclassified	21. NO. OF PAGES 18
		20. SECURITY CLASS (This page) Unclassified	22. PRICE

NOTICE

This document has been reviewed in accordance with U.S. Environmental Protection Agency policy and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Abstract

The National Acid Precipitation Assessment Program (NAPAP) has charged its Task Group on Emissions and Controls with the development of inventories of acid rain precursor emissions from anthropogenic sources. In order to support applications of the Eulerian Regional Acid Deposition Model (RADM), the 1980 NAPAP Annual Emissions Inventory was further resolved. Temporal allocation of annual emissions to hourly emissions estimates for a typical weekday, Saturday, and Sunday in each season; spatial allocation of county-level area source and minor point source emissions to 63,000 20 x 20 km grid cells; and species allocation of NO_x to NO and NO_2 , TSP to alkalinity classes, and VOC to 29 photochemical reactivity classes were performed. This paper describes the processes and data sources used to develop the NAPAP temporal, spatial, and species allocation factors.

Introduction

The National Acid Precipitation Assessment Program's (NAPAP) Task Group on Emissions and Controls is charged with the development of inventories of acid rain precursor emissions from anthropogenic sources. One of the most extensive uses of the 1980 NAPAP Emissions Inventory is to support applications of the Eulerian Regional Acid Deposition Model (RADM). To support Eulerian modeling applications, the 1980 NAPAP Annual Emissions Inventory (Version 5.0) had to be further resolved temporally, spatially, and by component species. Annual emissions had to be allocated to hourly emissions estimates for a typical weekday, Saturday, and Sunday in each season; county-level area source and minor point source emissions had to be spatially resolved to modeling grid cells; NO_x emissions had to be split into NO and NO_2 ; TSP emissions had to be assigned to alkalinity classes; and VOC emissions had to be apportioned into 29 photochemical reactivity classes.

To create the 1980 NAPAP Eulerian Modeling Emissions Inventory (Version 5.2), sets of temporal, spatial, and species allocation factors were developed and applied to the NAPAP Annual Emissions Inventory. The contents of the 1980 NAPAP Eulerian Modeling Emissions Inventory are presented in Table 1. This paper describes the processes and data sources used to develop the modeling data.

Temporal Allocation

The RADM requires hourly emissions data reflecting a complete 24-hour diurnal pattern for a typical weekday, Saturday, and Sunday in each season. Separate modeling files were created for each of the 12 temporal scenarios by developing and applying sets of seasonal, daily, and hourly fractions to the annual emissions data.

U.S. Area Source Temporal Allocation

Since the temporal distribution of emissions most often reflects the temporal patterns of anthropogenic activities which create the emissions, area source temporal allocation factors were derived for each of the 88 area source

TABLE 1. CONTENTS OF THE 1980 NAPAP EULERIAN
MODELING EMISSIONS INVENTORY

TEMPORAL RESOLUTION:	Hourly emissions values for a typical weekday, Saturday, and Sunday for all four seasons	
GEOGRAPHIC DOMAIN/RESOLUTION:	48 States and Canada; separate major point source file with minor point sources and area sources assigned to 63,000 20 x 20 km grid cells	
POLLUTANTS	SO ₂	VOC (cont.):
	SO ₄	- Isobutene
	TSP:	- Trans-2 butene
	- Ca	- Pentane
	- Mg	- Isopentane
	- K	- 2,3-dimethylbutane
	- Na	- Other alkenes
	Pb	- Other alkanes
	CO	- Formic acid
	HCl	- Acetic acid
	HF	- Other organic acids
	NO	- Formaldehyde
	NO ₂	- Acetaldehyde
	NH ₃	- Propionaldehyde
	VOC:	- Acetone
	- Methane	- Other ketones
	- Ethane	- Other aldehydes
	- Ethylene	- Xylene
	- Propane	- Benzene
	- Propylene	- Toluene
	- N-butane	- Ethylbenzene
	- 1,2-butene	- Other aromatics
	- Isobutane	

categories contained in the NAPAP Emissions Inventory based primarily on published activity statistics relating to each category. For example, seasonal, daily, and hourly patterns in residential fuel use were derived based on heating degree day data.¹ A representative meteorological station was chosen in each state; seasonal allocation factors were derived based on monthly average degree day data, and 3-hour temperature records were used to generate hourly patterns.

Similar methodologies were utilized to generate temporal allocation factors for the remaining categories drawing on data sources such as the U.S. Department of Transportation's continuous traffic count data,² the Federal Aviation Administration's air traffic data,³ the Bureau of Labor Statistics' data on working hours,⁴ and the U.S. Department of Transportation's data on gasoline sales.⁵ Where published activity data were unavailable, patterns were based on discussions with representatives of trade associations. Where such data or sources were unavailable, patterns from similar studies were used or engineering judgment was employed.

U.S. Point Source Temporal Allocation

For electric utilities in the Eastern United States, State and Source Classification Code (SCC) specific hourly temporal allocation factors were developed based on hourly power plant fuel use data previously collected for use in EPRI's SURE program.⁶ Regional average data from The EPRI Regional Systems⁷ were used to develop patterns for the rest of the United States.

Numerous studies describing nonutility point source temporal variations were examined, but generalized temporal factors for these other industries were not developed. The temporal factors described in these studies were found to be generally plant-specific and appropriate generalizations could not be made regarding applicability to broad industry classes. Rather, point-specific patterns were developed independently for every point source contained in the NAPAP Eulerian Modeling Emissions Inventory's major source file. In this context, major sources are those emitting more than 100 tons/year of any pollutant. Seasonal, daily, and hourly temporal patterns were derived based on operating pattern data contained in each point source record.

Canadian Temporal Allocation Factors

Canadian temporal allocation factors were developed separately under the auspices of Supply and Services Canada and adopted without substantial change for incorporation into the NAPAP Emissions Inventory. The Canadian temporal allocation factors were developed using methods similar to those used in the development of the U.S. factors. Business and government statistics and meteorological data were utilized as appropriate.

Where available data enabled such resolution, factors were developed at the province level. Where emissions were deemed to be climate dependent, an attempt was made to refine province-level factors further into latitude zones. The Canadian temporal factors were reviewed for consistency and reformatted for use in NAPAP.

Since the NAPAP study area spans several time zones, a file of time zone offset factors was created to adjust each temporal pattern to Greenwich Mean Time (GMT). Offsets were also developed to account for Daylight Savings Time in appropriate seasons in applicable areas.

Spatial Allocation

The NAPAP modeling grid system is comprised of 63,000 grid cells (210 rows, 300 columns) dimensioned 1/6-degree latitude by 1/4-degree longitude (approximately 20 x 20 km). The study area covers the 48 contiguous United States and most of Canada and extends from 50 to 125 degrees West longitude and from 25 to 60 degrees North latitude.

Point source records contain locational information making their assignment to grid cells straightforward. Latitude and longitude locational data were used to assign each point source to the appropriate grid cell. Area source emissions data, compiled on a county basis, were apportioned to grid cells using spatial allocation factors, fractional multipliers that assign a portion of a county's emissions to a particular grid cell. Generally, since the subcounty distribution of emissions is unknown, emissions are apportioned on the basis of some surrogate indicator.

Spatial allocation factors were derived for population, housing, land area, 10 land-use categories, and one composite land-use category. The separately developed spatial allocation factor files were then merged into a single file for use in generating the modeling tapes. The development of each set of allocation factors is described below.

Housing and Population

The U.S. Bureau of the Census maintains information on the distribution of housing and population at several levels of detail. 1980 Census data, available as part of EPA's STF3A Census Tapes, were utilized to derive spatial allocation factors for the surrogates of housing and population. Based on an analysis of available data resolution compared to the NAPAP modeling grid cell size, population and housing data at the census tract level were utilized. Based on the location of the geographic centroid of each census tract, county level populations and housing counts were allocated to grid cells. The county-to-grid allocation factors for these two surrogates were computed as the fraction of a given county's population or housing units that fell within a grid cell.

Some anomalies in the census and emissions data had to be taken into account in this process. For example, some localities repress portions of their housing and population data to maintain confidentiality, and some inconsistencies were encountered between the census and emissions data regarding cities that are treated as independent "county equivalents." The Commonwealth of Massachusetts maintains area source emissions data on the basis of Air Pollution Control Districts, which do not adhere to county boundaries. Each of these special cases dictated appropriate deviations from the basic methodology.

Land Use

Land-use data, derived from Landsat mosaic images,⁸ were obtained and contain 10 land-use/cover percentages for each NAPAP grid cell. Each land classification percentage represents the fraction of that grid cell comprised of each land-use/cover category. The Landsat data were used with grid/county land area relationships to derive spatial allocation factors:

$$SPAFCT_{CS1} = \frac{(A_{C1}) (A_{S1})}{\sum_1^n (A_{C1}) (A_{S1})}$$

where: $SPAFCT_{CS1}$ = The spatial allocation factor for county C, land-use type S, and grid 1

A_{C1} = The portion of county C that falls within grid 1

A_{S1} = The fraction of grid 1 with land-use type S

n = The total number of grids covering county C

The land-use allocation factors were merged with the land area, population, and housing allocation factors, providing a total of 14 possible spatial allocation surrogates. The final step in spatially allocating county-level emissions to grid cells was to assign the most appropriate surrogate to each of the 88 area source categories.

Species Allocation

To support applications of the RADM, three of the pollutants in the NAPAP Annual Emissions Inventory, NO_x , TSP, and VOC, had to be further refined: NO_x emissions had to be split into NO and NO_2 ; TSP emissions had to be assigned to alkalinity classes; and VOC emissions had to be broken down by photochemical reactivity class.

Profiles of NO_x emissions, referenced by SCC, were developed using patterns previously derived for the SURE and Northeast Corridor Regional Modeling Project (NECRMP)⁹ emissions inventories. Alkaline dust emission factors were similarly used to apportion TSP into five alkalinity classes.

There are numerous possible VOC speciation schemes based on different modeling chemistries. Since the modelers desire the flexibility to test a number of possible chemistries, a more complex approach was necessary for VOC emissions. Using primarily published information,¹⁰ sets of species profiles were developed. Each profile provides a breakdown of a category's VOC emissions into a typical set of component species. Each of the 160 individual species is defined by its SAROAD code, molecular weight, and weight percent of total VOC emissions. By distributing emissions to individual species, the profiles become independent of any particular reactivity scheme, and may be manipulated into any reactivity classification.

To "speciate" emissions, two additional files were employed. An SCC index file links each SCC in the inventory with the appropriate species profile. Next, a class assignments file assigns each of the 160 independent species to one of the 29 photochemical classes currently being utilized in the RADM.

Eulerian Modeling Files

To enable generation of the modeling input files from the NAPAP Annual Emissions Inventory, a data handling system was designed and implemented. The Flexible Regional Emissions Data Systems (FREDS), consisting of five primary independent subsystems written in the command language of the Statistical Analysis System (SAS), was utilized to generate 12 modeler's tapes which together represent Version 5.2 of the NAPAP Emissions Inventory. Each of the 12 temporal scenarios described earlier is represented by an independent modeler's tape. Figure 1 shows the relationship of each of the allocation factor files and corresponding FREDS module.

Results

Hourly emissions of SO_2 , NO_x , and VOC for a typical summer weekday, nationwide are shown in Figure 2. Figure 3 shows the distribution of annual emissions of VOC into photochemical reactivity classes. The distribution of annual NO_x emissions into NO and NO_2 is shown by EPA Region in Figure 4, while Figure 5 presents SO_2 and SO_4 emissions by EPA Region. Spatial distributions of SO_2 , NO_x , and VOC emissions are shown in Figures 6 through 8, respectively.

Summary

This paper has described the development of the NAPAP Eulerian Modeling Emissions Inventory for the 1980 base year. Development of the allocation factors and corresponding data handling system has been covered. Although developed specifically to drive applications of the RADM, the input allocation factor files and data handling system can easily be adapted to address the needs of other similar regional-scale atmospheric simulation modeling programs as well.

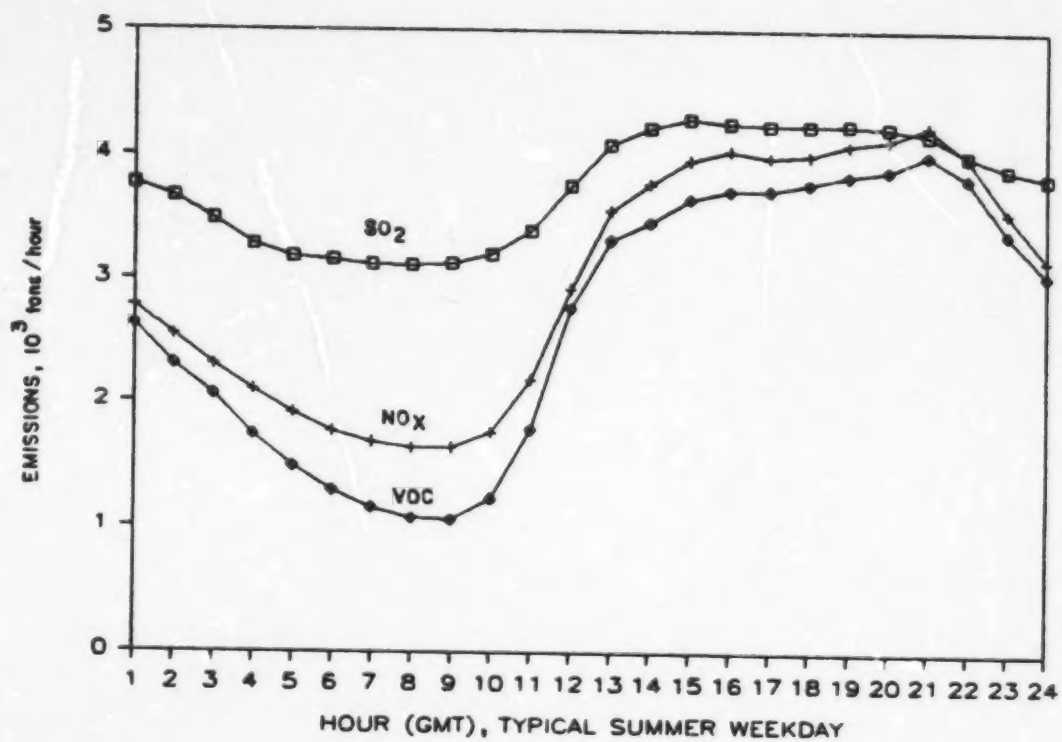
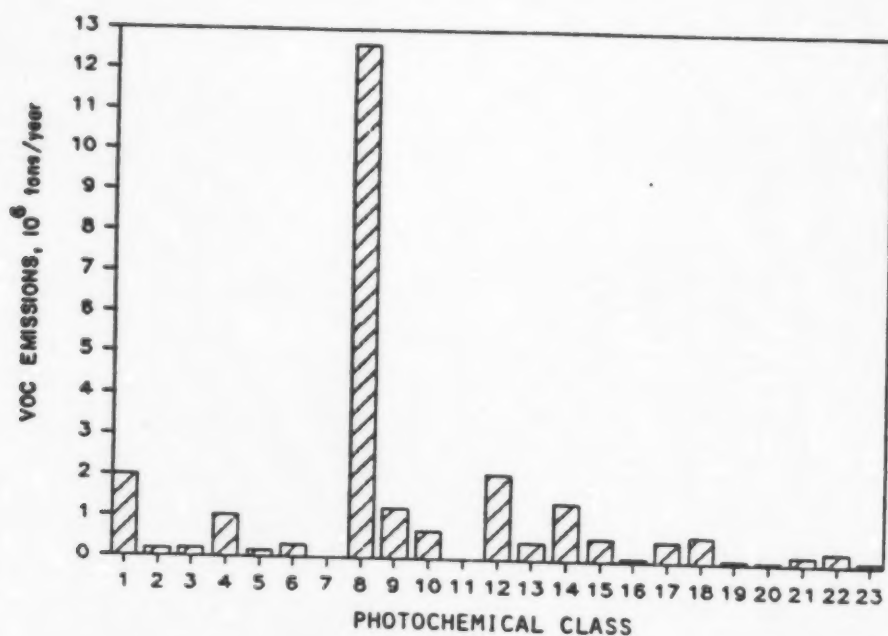


Figure 2. Diurnal emissions pattern for a typical summer weekday, 1980 NAPAP Emissions Inventory.



VOC CLASS NO.	VOC CLASS NAME*
------------------	--------------------

1	METHANE
2	ETHANE
3	PROPANE
4	BUTANE
5	ISO-BUTANE
6	PENTANE
7	ISO-PENTANE
8	OTHER ALKANES
9	ETHYLENE
10	PROPYLENE
11	ISO-BUTENE
12	OTHER ALKENES
13	BENZENE
14	TOLUENE
15	XYLENE
16	ETHYL BENZENE
17	OTHER AROMATICS
18	FORMALDEHYDE
19	ACETALDEHYDE
20	OTHER ALDEHYDES
21	ACETONE
22	OTHER KETONES
23	ORGANIC ACIDS

*The following photochemical reactivity classes have no emissions: 1,2-butene, trans-2-butene, 2,3-dimethylbutane, formic acid, acetic acid, and propionaldehyde.

Figure 3. Distribution of annual VOC emissions into photochemical reactivity classes, 1980 NAPAP Emissions Inventory.

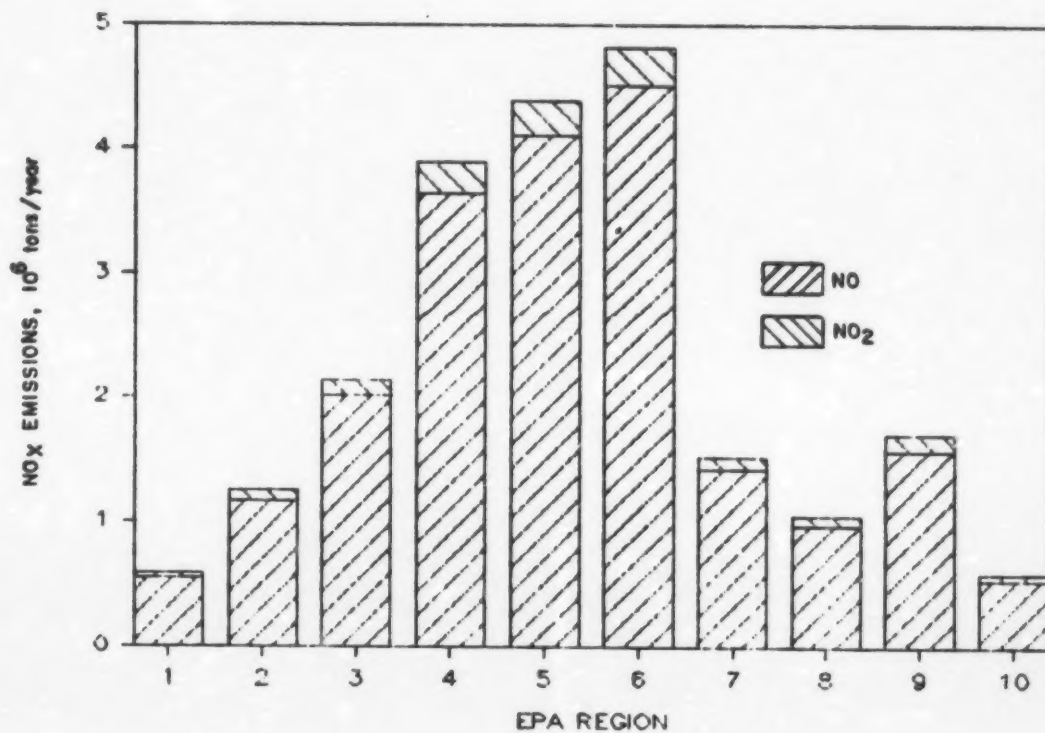


Figure 4. Annual NO_x emissions by EPA Region, 1980 NAPAP Emissions Inventory.

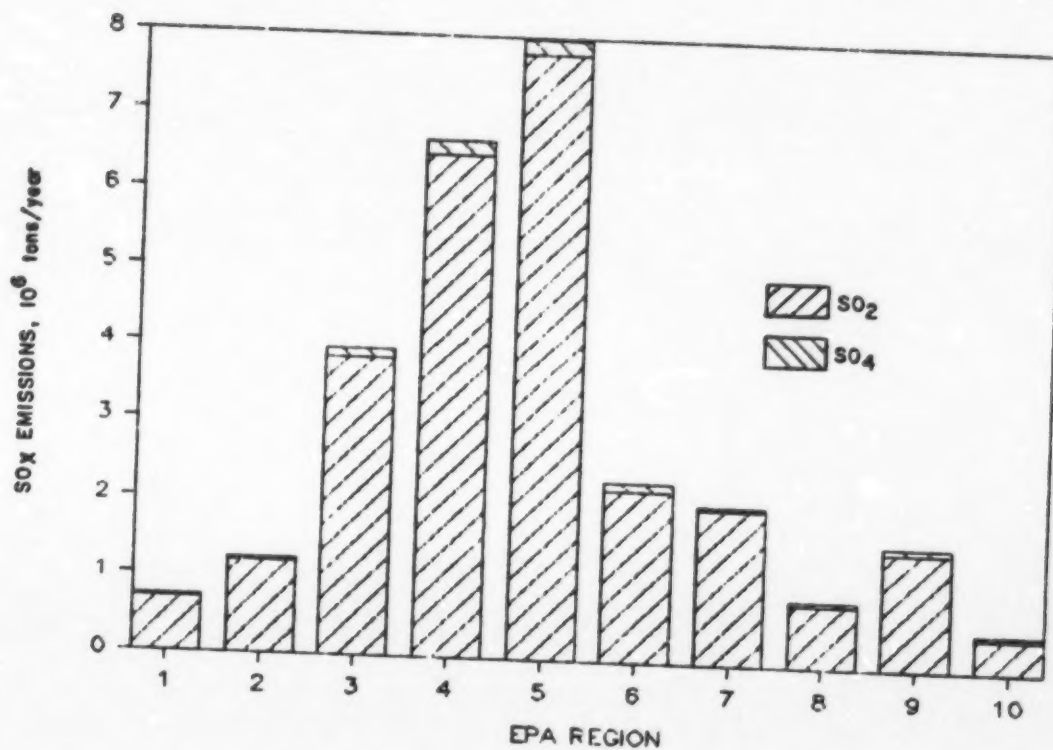


Figure 5. Annual SO_x emissions by EPA Region, 1980 NAPAP Emissions Inventory.

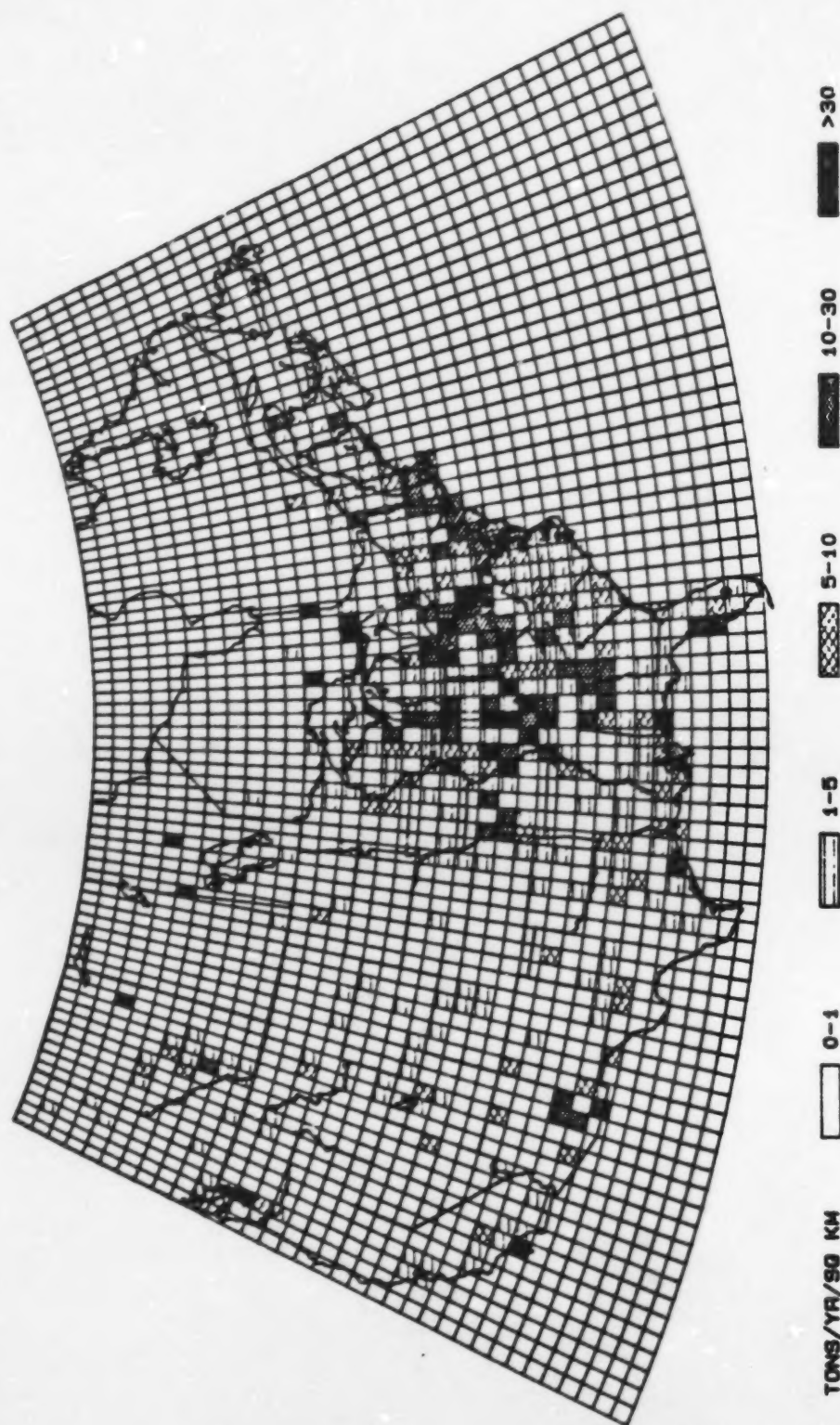


Figure 6. SO₂ Emission density, 1980 NAPAP Emissions Inventory.

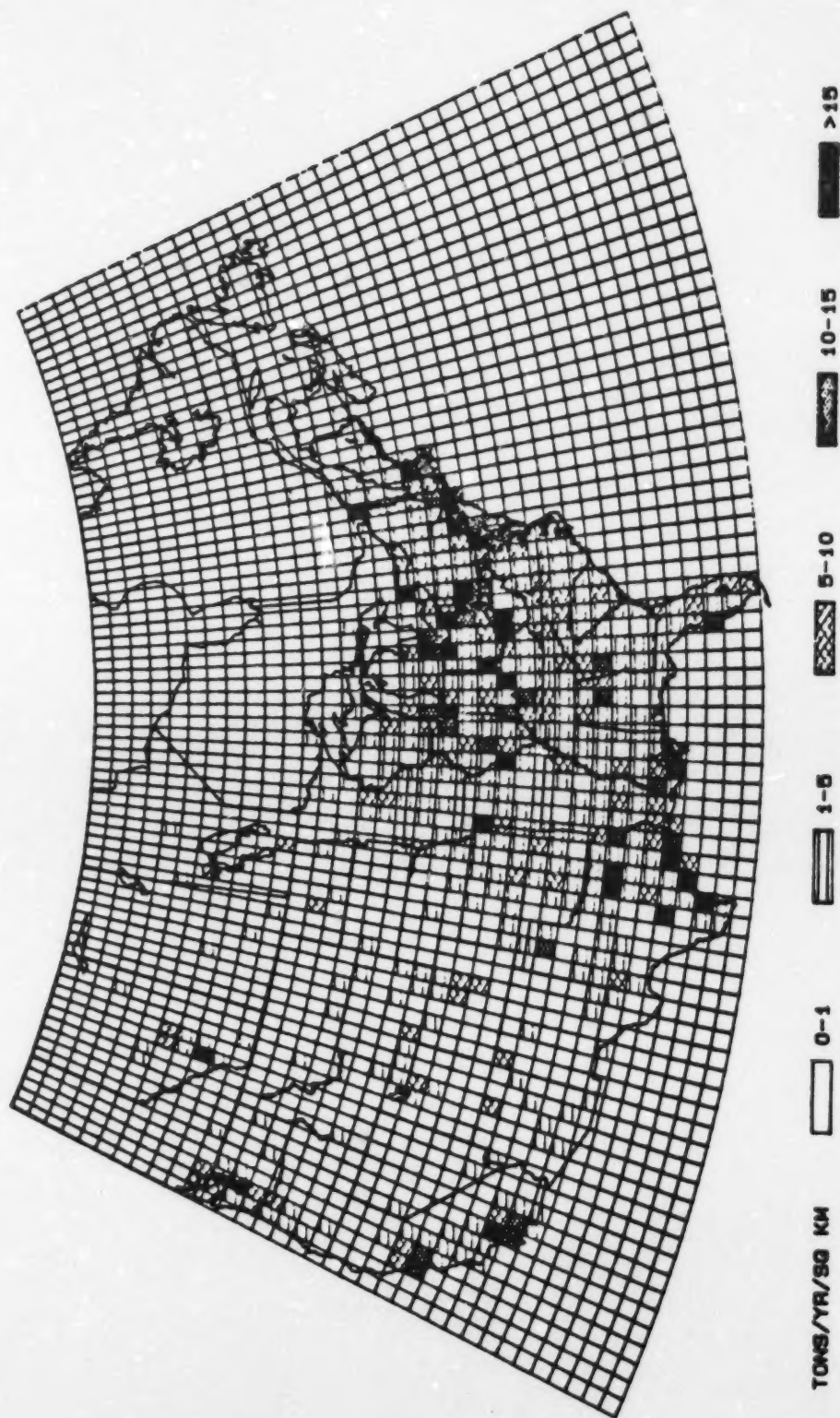


Figure 7. NO_x Emission density, 1980 NAPAP Emissions Inventory.

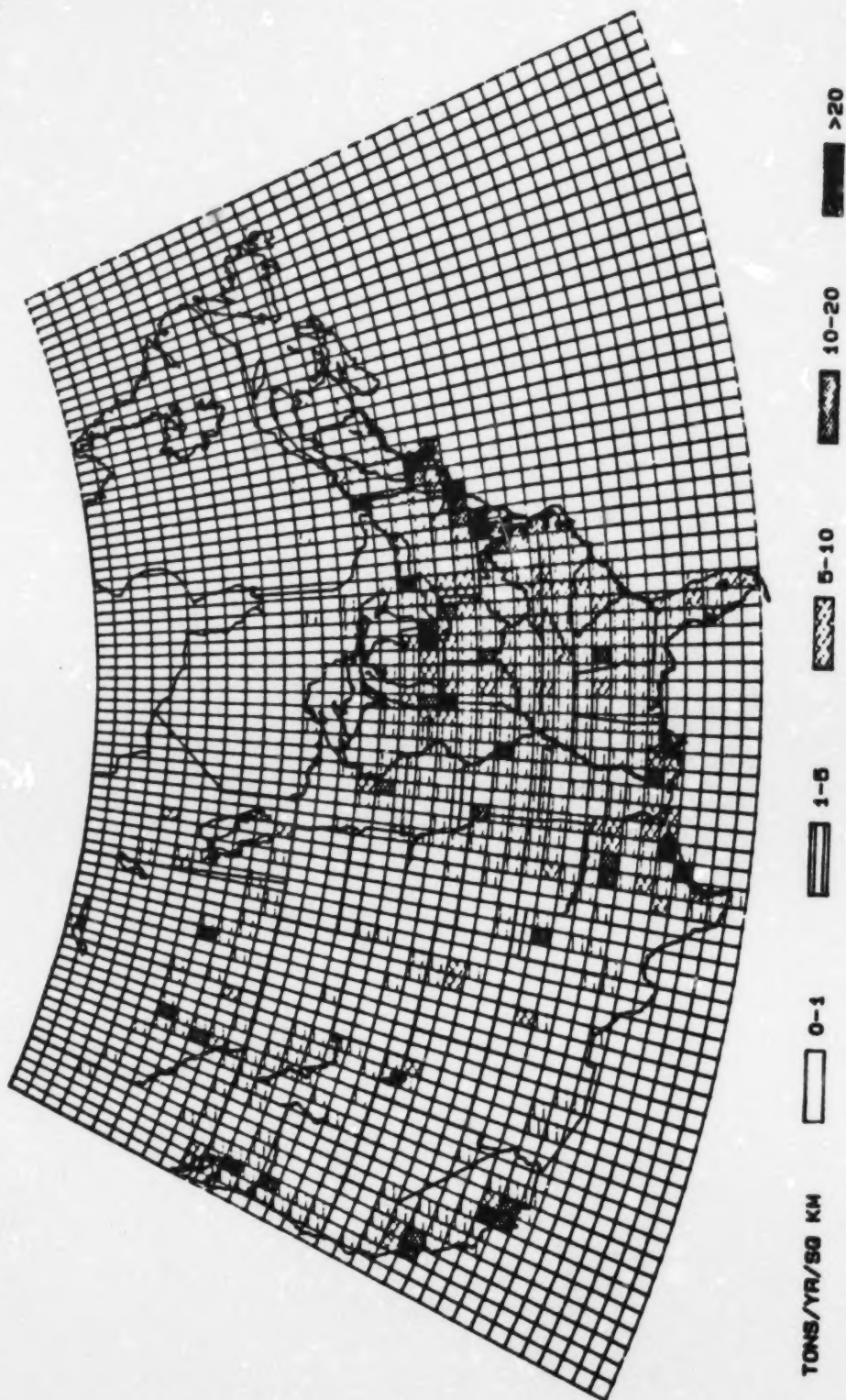


Figure 8. VOC Emission density, 1980 NAPAP Emissions Inventory.

References

1. National Climatic Data Center (NCDC), National Oceanic and Atmospheric Administration (NOAA). Local Climatological Data Published Stations (1980 data). Asheville, North Carolina.
2. U.S. Department of Transportation. Continuous Traffic Count Data for 1980. Washington, DC.
3. Seasonally Adjusted Traffic and Capacity. U.S. Civil Aeronautics Board, Washington, DC. July 1981.
4. U.S. Department of Labor, Bureau of Labor Statistics. Supplement to Employment and Earnings: Revised Establishment Data. August 1981.
5. Highway Statistics 1980. U.S. Department of Transportation, Federal Highway Administration, Washington, DC.
6. Klemm, H. A. and R. J. Brennan. Emissions Inventory for the SURE Region. GCA/Technology Division for the Electric Power Research Institute (EPRI). EA-1913. April 1981.
7. Mulvaney, J. J. The EPRI Regional Systems. Electric Power Research Institute, Palo Alto, California. P-1950-52. July 1981.
8. S. H. Page, National Land Use and Land Cover Inventory, Lockheed Engineering and Management Services Company for the U.S. EPA, Office of Research and Development, Las Vegas, NV, April 1980.
9. Sellers, F. M., M. J. Geraghty, A. M. Kiddie, B. J. Bosy, and S. V. Capone. The Northeast Corridor Regional Modeling Project Annual Emission Inventory Compilation and Formatting--Volume XVII--Development of Temporal, Spatial and Species Allocation Factors. EPA-450/4-82-013q. October 1982.
10. Volatile Organic Compound (VOC) Species Data Manual, Second Edition. U.S. EPA, Office of Air, Noise, and Radiation, Office of Air Quality Planning and Standards, EPA-450/4-80-015, July 1980.

Acknowledgment

GCA was funded for this effort under EPA Contract 68-02-3997, Work Assignment 13. This activity was administered by EPA in association with the National Acid Precipitation Assessment Program.